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Correlation of optical conductivity and angle-resolved photoemission spectra of strong-coupling large polarons and its display in cuprates

A. E. Myasnikova and E. N. Myasnikov
South Federal University, 344090 Rostov-on-Don, Russia

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A common approach is used to calculate a band due to strong-coupling large polaron (SCLP) photodissociation in angle-resolved photoemission spectroscopy (ARPES) and in optical conductivity (OC) spectra. It is based on using the coherent-state representation for the phonon field in SCLP. The calculated positions of both band maxima are universal functions of one parameter—the SCLP binding energy E_p: a maximum of the band in the ARPES spectrum lies at a carrier binding energy of about $3.2E_p$; the OC band maximum is at a photon energy of about $4.2E_p$. The half-widths of the bands are mainly determined by E_p and slightly depend on the electron-phonon coupling constant α; for $\alpha=6-8$, the half-width of the band in the ARPES spectrum is $1.7-1.3E_p$ and the OC band half-width is $2.8-2.2E_p$. By using these results, one can predict the approximate maximum position and half-width of the band in the ARPES spectrum from the maximum of the mid-IR OC band and vice versa. Comparison of the results with experiments leads to the conclusion that underdoped cuprates contain SCLPs with $E_p=0.1-0.2$ eV, which is in good conformity with the medium parameters in cuprates. The values of the polaron binding energy determined from experimental ARPES and OC spectra of the same material are in good conformity, too: the difference between them is within 10%.

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I. INTRODUCTION

Angle-resolved photoemission spectroscopy (ARPES) as well as ooptical conductivity (OC) spectra of underdoped high-temperature superconductors and other complex oxides demonstrate broad bands[1–17] naturally interpreted[1–3] as caused by strong-coupling polarons. Strong-coupling polaron is formed by a charge carrier in a strongly polarizable medium, i.e., in a system with strong electron-phonon interaction. In the case of strong electron-phonon interaction, the average number of phonons accompanying the charge carrier that can be estimated as $E_p/\hbar\omega$ (where E_p is the polaron binding energy and $\hbar\omega$ is the phonon energy) is much higher than unity. Strong-coupling polaron is qualitatively different from weak-coupling polaron (corresponding to the opposite case $E_p/\hbar\omega<1$), which is a state with a certain momentum, similar to a carrier state in the absence of electron-phonon interaction, but its effective mass is modified due to this interaction. Strong-coupling polaron is a state with spontaneous break of the system translational symmetry[18]: the charge carrier is localized in a polarization potential well formed due to electron-phonon interaction. In such a state, the phonon field has nonzero average values of shift in all harmonics or in most of the harmonics, i.e., it is in a quantum-coherent state.[19] The quantum-coherent state is characterized by an uncertain number of quanta in each harmonics but sufficiently well defined phase of harmonics.[20]

There are two types of strong-coupling polarons. The ratio of the width of the bare-carrier band to the polaron binding energy E_p separates the cases of large polaron and small polaron. In the case of a narrow bare-carrier band (when the ratio is less than unity), the carrier localization in one elementary cell does not lead to a large increase in its kinetic energy and a small polaron is formed.[21,22] In the case of a wide bare-carrier band, a strong-coupling large polaron (SCLP) spreading over several elementary cells occurs.[22] As a result, SCLP can move without any activation, which is in contrast to a small polaron. This causes the high mobility of SCLPs similar to that observed in cuprates.[1]

Obviously, since both kinds of strong-coupling polarons (large and small) include the coherent state of the phonon field, their photodissociation will be accompanied by the appearance of a sufficiently large number of phonons different in different acts due to the uncertainty in the number of quanta in each harmonics. This is displayed in the so-called phonon sidebands[1–3] observed in the ARPES and OC spectra of underdoped cuprates and other complex oxides. Several groups calculated ARPES spectra caused by small polarons in the frames of the *t*-*J* model.[3,23] The width of the band that they obtained is in good conformity with experiment, which is in contrast to its energetical position: the calculated band maximum corresponds to a carrier binding energy of about 1.2 eV, which is much higher than that in experiments [0.5–0.6 eV (Refs. 1–6)]. The ARPES spectrum caused by photodissociation of SCLPs was not calculated earlier but since their binding energy is smaller than that of small polarons, one can hope to obtain a band that will be in good conformity with experiments.

Optical conductivity (or optical absorption) caused by SCLPs was calculated by several groups with essentially different results. The calculation in Refs. 24 and 25 yields the band with the maximum at approximately SCLP binding energy E_p. Experimental mid-IR bands in OC spectra of complex oxides have maxima at 0.5–0.8 eV.[7–17] By supposing that these values are SCLP binding energies, they turn out to be much greater than that estimated according to the SCLP theory[26] used for typical cuprate medium parameters. Pekar[27] and Emin[22] considered an absorption spectrum caused by photodissociation of SCLPs and predicted the band with the maximum at approximately $3E_p$. The reason of ambiguity in predictions of the OC spectrum caused by SCLPs is the two different possible consequences of photon absorption by

SCLP. It can appear in an excited state where the charge carrier is still coupled with the polarization potential well or the charge carrier can leave the well and the well decays (photodissociation of SCLP).

The maximum of the absorption band obtained by Pekar[27] and Emin[22] (at about $3E_p$) is in sufficiently good conformity with experimental OC spectra. (That is, the polaron binding energy estimated as one-third of the energy of band maximum is in good conformity with that calculated according to the SCLP theory[26] applied to medium parameters typical for cuprates.) However, the form of the band predicted in Ref. 22 (strongly asymmetric with an almost vertical low-energy edge) differs from the results of experiments. The processes of internal photoelectric effect and photoemission are sufficiently similar, as noted by Emin,[22] and we will use this similarity to find correlation in the ARPES and OC spectra caused by SCLP photodissociation.

Photodissociation is the breaking of polaron due to photon absorption. The transverse electromagnetic field of a photon does not interact with the longitudinal polarization field constituting SCLP; it affects only the charge carrier. According to the adiabatic condition satisfied in the SCLP case ($E_p/\hbar\omega \gg 1$,[27] where $\hbar\omega$ is the phonon energy), the photodissociation time [approximately $\hbar/(3E_p)$ (Refs. 22 and 27)] is much shorter than the characteristic phonon time ω^{-1}. Therefore, the phonon field does not have the time to dress the charge carrier with a polarization cloud during the time of carrier phototransition, and the state of the phonon field does not change during this time, which is in conformity with the Franck–Condon principle.[22,24,25,27] Thus, at the SCLP photodissociation, the electron released by the photon from the potential well appears in one of the states of the continual energy spectrum. We will approximate the carrier states in the continual spectrum as plane waves. In the case of photoemission when the photon energy is of the order of tens of eV, this approximation is ordinary. In the case of optical conductivity, we can check the applicability of this approximation by comparing the result of calculation with experiments. We demonstrate below that the values of the polaron binding energies determined from experimental ARPES and OC spectra of the same material according to expressions obtained coincide (the difference between them is smaller than 10%.)

Emin proposed such approach (approximation of final carrier states after SCLP photodissociation with plane waves) in the calculation of optical absorption in Ref. 22. However, following Pekar,[27] he used a classical description for the polarization field in SCLP. In this approach, the polarization field energy (and, hence, the number of radiated phonons) is fixed ($2E_p$). Accordingly, Pekar[27] predicted that optical dissociation of SCLP takes three times its binding energy, which is in contrast to its thermal dissociation, which takes only E_p. In conformity with this prediction, the maximum of the band in the absorption spectrum calculated by Emin[22] is situated at about $3E_p$. The band has some half-width due to the different possible values of the carrier momentum.

In contrast to the work of Emin,[22] we consider the polarization field in SCLP quantum-mechanically[18,28] by using the quantum-coherent-state representation. It is shown in Ref. 18 that the SCLP includes the coherent lattice deformation. It is coordinated in the phase superposition of the lattice states with different numbers of phonons so that one can call it a phonon condensate. Since for the phonon part of SCLP its photodissociation is quick, a Franck–Condon process,[22,24–26] the phonon condensate spontaneously decays (without participation of the electron-phonon interaction) when the charge carrier has left the potential well. The quantum-coherent state can be expanded in terms of states with a certain number of phonons[19]; the expansion contains summands with all possible numbers of quanta. Therefore, decay of the coherent part of the polarization field at the SCLP photodissociation is accompanied by radiation of a random number of phonons in each event. Only the average energy of phonons radiated in a single act is $2E_p$. As a result, the corresponding band in the OC spectrum is wider and more symmetrical than that calculated with classical consideration of the polarization field, and the position of its maximum ($4.2E_p$) differs from the predictions of classical theory ($3E_p$).

It should be noted that our consideration of the ARPES spectrum does not take into account the electron losses at crossing the crystal. In the OC spectrum, we do not calculate the part of the spectrum caused by the charge carrier transitions into polaronic relaxed excited states (states of the discrete energy spectrum). This part of the OC spectrum of SCLP was calculated in Refs. 24, 25, and 29. To obtain the complete OC spectrum of SCLP, one should unite the band caused by SCLP photodissociation calculated here, the band caused by transitions into polaronic states, and the Drude contribution.

It is interesting to note that such a complex structure is demonstrated by the polaronic OC spectrum only in the case of strong electron-phonon coupling. In the case of weak and intermediate electron-phonon couplings, the band caused by the polaron photodissociation is absent. The reason for this difference is the fact that separation of the polaron at the phototransition into two uncoupled parts can occur only in the case of strong electron-phonon coupling. In the weak- and intermediate-coupling cases, the Franck–Condon principle is not applicable so that the electron transition into a new state after the photon absorption is accompanied by a change in the lattice state. Indeed, in this case, the time of the phototransition is of the same order as the characteristic phonon time ω^{-1}. Therefore, because of the photon absorption, the weak- and/or intermediate-coupling polaron passes again into a polaron state (a state of the electron coupled with phonons but not self-consistent at first[29]). That is, the photodissociation of the polaron in the weak- and intermediate-coupling cases cannot occur.

Thus, we suggest a sufficiently simple and apparent method of calculating the band in ARPES and OC spectra caused by SCLP photodissociation. The method is based on using the coherent-state representation for the state of the phonon field in SCLP. Parameters of the coherent state of the polarization field as function of the medium parameters are obtained in Ref. 18 by variation. Then, the Fermi golden rule is applied to calculate the probability of the SCLP photodissociation resulting in radiation of different numbers of phonons.[28] This probability allows the calculation of the band caused by SCLP photodissociation in both ARPES and OC spectra.

II. BAND IN ANGLE-RESOLVED PHOTOEMISSION SPECTROSCOPY AND OPTICAL CONDUCTIVITY SPECTRA CAUSED BY STRONG-COUPLING LARGE POLARON PHOTODISSOCIATION

Let us briefly recall the calculation of the probability of the SCLP photodissociation with radiation of v phonons[28] and then use it to obtain bands in ARPES and OC spectra caused by SCLP photodissociation. The probability W_{if} of the system transition from the initial state $|i\rangle$ into the state $|f\rangle$ per unit time under the influence of the operator $\hat{H}_{\text{int}}$ according to the Fermi golden rule is

$$W_{if} = \frac{2\pi}{\hbar}|\langle f|\hat{H}_{\text{int}}|i\rangle|^2 \delta(E_i - E_f), \tag{1}$$

where E_i and E_f are the energies of the initial and final states of the system. The polaron photodissociation occurs as a result of interaction of an electromagnetic wave of frequency Ω with the charge carrier in the polaron (the longitudinal field of the polarization in the polaron obviously does not interact with the transverse electromagnetic wave). The operator of the interaction has the following form:

$$\hat{H}_{\text{int}} = \frac{e\hbar(\mathbf{kA})}{m^* c} e^{i\mathbf{Q}\cdot\mathbf{r}}, \tag{2}$$

where $\hbar\mathbf{k}$ is the electron momentum and $\mathbf{A}$ is the amplitude of the vector potential of the electromagnetic field, which is related to its intensity I as follows: $I = \Omega \mathbf{A}^2/2\pi\hbar c$; $\mathbf{Q}$ is the wave vector of the electromagnetic wave.

At $T=0$ K, the initial state of the system is the ground state of the polaron in an electromagnetic field with frequency Ω. Therefore, the initial state and its energy are

$$|i\rangle = \sqrt{\beta^3/7\pi}(1+\beta r)\exp(-\beta r)\prod_{\text{q}} |d_{\text{q}}\rangle, \tag{3}$$

and $E_i = -E_p + \hbar\Omega$, respectively, where the Pekar[27] wave function for the carrier state in the polaron is used. The parameters $d_{\mathbf{k}} = |d_{\mathbf{k}}| e^{i\phi_{\mathbf{k}}}$ of the coherent state of the phonon field in a ground state of SCLP found by the variation in Ref. 18 have the following form:

$$|d_{\mathbf{k}}| = \frac{e}{|\mathbf{k}|}\sqrt{2\pi}(V\varepsilon^* \hbar\omega_{\mathbf{k}})^{1/2}\eta_{\mathbf{k}}(\beta), \tag{4}$$

$$\varphi_{\mathbf{k}} = -\mathbf{kR} + 2\pi C(\mathbf{kR}), \tag{5}$$

where V is the crystal volume, ω_k is the phonon frequency, $\eta_{\mathbf{k}}(\beta)$ is the Fourier transform of the square of modulus of the carrier wave function in the polaron, β is the parameter characterizing the degree of the carrier localization in the polaron, $\mathbf{R}$ is the coordinate of the polaron center, and $C(\mathbf{kR})$ is an integer chosen in such a way that the phase $\varphi_{\mathbf{k}}$ belongs to the interval $[-\pi, +\pi]$.

Photodissociation of SCLP is a Franck–Condon process since, according to the adiabatic condition satisfied in the strong-coupling case, the polaron binding energy E_p is much larger than the phonon energy $\hbar\omega$. Then, the carrier phototransition time [in the case of strong-coupling large polaron, it is about $\hbar/3E_p$ (Refs. 22 and 27)] is much shorter than the characteristic phonon time ω^{-1}. Thus, decay of the polaronic phonon "cloud" occurs without participation of electron-phonon interaction. The vectors of the possible final states of the phonon field are a superposition of eigenvectors, $|\{\nu_{\text{q}}\}\rangle = \Pi_{\text{q}}|\nu_{\text{q}}\rangle$, of the nonshifted Hamiltonian, $\hat{H}_{\text{ph}} = \Sigma_{\text{q}}\hbar\omega_{\text{q}} b_{\text{q}}^+ b_{\text{q}}$, describing the states with a certain number of quanta ν_{q} in each harmonics. The electron final state after SCLP photodissociation, as we discussed in the Sec. I, is a free-carrier state not coupled with the polarization potential well and can be approximated as a plane-wave state. Thus, after photodissociation, the state [Eq. (3)] transforms into

$$|f\rangle = L^{-3/2}\exp(i\mathbf{kr})\prod_{\text{q}} |\{\nu_{\text{q}}\}\rangle, \tag{6}$$

provided that the sum of ν_{q} (taking the value 0 or 1) from the set $\{\nu_{\text{q}}\}$ yields a certain number ν. Hence, the energy of the final state is $E_f = \hbar^2\mathbf{k}^2/2m^* + \hbar\omega\nu$ if we neglect the dependence of ω on $\mathbf{q}$, and

$$\delta(E_i - E_f) = \delta\left(-E_p + \hbar\Omega - \frac{\hbar^2\mathbf{k}^2}{2m^*} - \nu\hbar\omega\right). \tag{7}$$

The probability of the electron transition into a state with the wave vector with modulus k and direction in a spatial angle $d\Omega$ around the direction determined by angles φ, θ has the following form:

$$dW_{\{\nu_{\text{q}}\},\text{k}} = \frac{2\pi}{\hbar}\left\{\frac{e\hbar(\mathbf{kA})}{m^* c} 32\sqrt{\frac{\pi}{7\beta^3}} L^{-3/2} \times (1+\beta^{-2}|\mathbf{Q}-\mathbf{k}|^2)^{-3}\right\}^2 \cdot \prod_{\text{q}} |\langle \nu_{\text{q}}|d_{\text{q}}\rangle|^2 \times d\rho(\mathbf{k}), \tag{8}$$

where

$$d\rho(\text{k}) = \frac{m^* L^3 k(\varepsilon)}{(2\pi)^3\hbar^2} d\Omega$$

is the spectral density of the final carrier states with the wave vector directed in the body angle $d\Omega$.[22] According to expression (7), the electron momentum $\hbar$k and kinetic energy ε in the final state are related as follows:

$$\hbar k(\varepsilon) = \sqrt{2m^*\varepsilon} = \sqrt{2m^*(\hbar\Omega - E_p - \nu\hbar\omega)}. \tag{9}$$

According to the energy and the momentum conservation laws [expression (7) and $\mathbf{Q} = \mathbf{k} + \mathbf{q}_0$, where $\mathbf{q}_0$ is the wave vector of the phonon field after the polaron photoionization, $\mathbf{q}_0 = \Sigma_{\text{q}}\mathbf{q}\nu_{\text{q}}$), an experiment can measure only the probability [Eq. (8)] summarized over all possible sets $\{\nu_{\text{q}}\}$ with the same values of $\nu = \Sigma_{\text{q}}\nu_{\text{q}}$ and $\mathbf{q}_0$,

$$dW_{\{\nu_{\text{q}}\},\mathbf{k}} = \frac{2\pi}{\hbar}\left\{\frac{e\hbar(\mathbf{kA})}{m^* c} 32\sqrt{\frac{\pi}{7\beta^3}} L^{-3/2} \times (1+\beta^{-2}|\mathbf{Q}-\mathbf{k}|^2)^{-3}\right\}^2 \cdot \sum_{\{\nu_{\text{q}}\}}^{\nu} \prod_{\text{q}} |\langle \nu_{\text{q}}|d_{\text{q}}\rangle|^2 \times d\rho(\mathbf{k}). \tag{10}$$

Here, the symbol ν over Σ denotes that the sum is carried out over the sets $\{\nu_{\mathrm{q}}\}$ satisfying the condition $\Sigma_{\mathrm{q}}\nu_{\mathrm{q}}=\nu$. Besides, there is no set with $\nu=0$ among the sets $\{\nu_{\mathrm{q}}\}$. Indeed, in such a case, $\mathrm{q}_0=0$; hence, $\mathbf{k}=\mathbf{Q}$ and $\mathbf{kA}=\mathbf{QA}=0$, i.e., the probability of a transition with the appearance of such a set $\{\nu_{\mathrm{q}}\}$ is zero.

The sum in Eq. (10) expressing the probability of radiation of ν phonons in the SCLP photodissociation was calculated in Ref. 28,

$$P_\nu=\sum_{\{\nu_{\mathrm{q}}\}}\prod_{\mathrm{q}}^{\nu}|\langle\nu_{\mathrm{q}}|d_{\mathrm{q}}\rangle|^2=\frac{\bar{\nu}^{\nu-1}}{(\nu-1)!}e^{-\bar{\nu}},\tag{11}$$

where $\bar{\nu}$ is the average number of phonons radiated at the SCLP photodissociation,[28]

$$\bar{\nu}=2E_p(\hbar\omega)^{-1}.\tag{12}$$

To calculate the band in the ARPES spectrum caused by SCLP photodissociation, we use geometry which is ordinary for ARPES experiment,[1,2] where the wave vector $\mathbf{Q}$ of the incident photon lies in theXZ plane of the coordinate system and makes an angle ψ with the z axes. The XY plane of the coordinate system coincides with the sample surface. Wave vector $\mathbf{k}$ of the photoelectron inside the medium is considered to have a component $k_\parallel$ lying in the XY plane and $k_\perp$ in the perpendicular direction. The angle between $k_\parallel$ and the x axis is φ. As ARPES measures the energy ε' and momentum k' of the electron outside the medium, we should express the probability [Eq. (10)] in terms of these variables. According to energy conservation law,[1,2] the electron kinetic energy outside the medium is

$$\varepsilon'=\frac{\hbar^2k'^2}{2m_e}=\varepsilon-\Phi=\hbar\Omega-\Phi-E_p-\nu\hbar\omega,\tag{13}$$

where Φ is the work function. The electron wave vector component lying in the XY plane $k_\parallel$ is continuous on the medium boundary.[1,2] The perpendicular component $k_\perp$ is discontinuous on the boundary.[1,2] If the dispersion of the electron inside and outside the medium differs only by its effective mass (m^* and m_e, respectively), then

$$k'_\perp=\sqrt{(2m^*\varepsilon'/\hbar^2)(m^*/m_e)-k_\parallel^2}$$

and

$$(\mathbf{kA})=k_\parallel\cos\varphi A\cos\psi+k'_\perp A\sin\psi.\tag{14}$$

The wave vector $\mathbf{Q}$ of photons ordinarily used in ARPES can be approximated as zero.[1,2]

Thus, expression (10) takes the following form:

$$dW_{\{\nu_{\mathrm{q}}\},\mathbf{k}}=\frac{256e^2}{7\pi\hbar m^*c^2\beta^3}\frac{[k_\parallel\cos\varphi\cos\psi+\sqrt{(2m^*\varepsilon'/\hbar^2)(m^*/m_e)-k_\parallel^2}\sin\psi]^2A^2k'}{(1+\beta^{-2}k'^2)^6}\cdot\frac{\bar{\nu}^{\nu-1}}{(\nu-1)!}e^{-\bar{\nu}}d\Omega,\tag{15}$$

where the body angle $d\Omega$ contains a factor $\sqrt{2m^*\varepsilon'/\hbar^2-k_\parallel^2}/k'_\perp$ due to $k_\perp$ discontinuity on the medium boundary and k' is determined by expression (13). Expression (15) represents the probability of the polaron photodissociation at $T=0$ K with the appearance of ν phonons and electron with the kinetic energy ε' and wave vector $\mathbf{k}'$ in the body angle $d\Omega$ around the direction determined by $\mathbf{k}'$ projections on the X, Y, and Z axes, $k_\parallel\cos\varphi$, $k_\parallel\sin\varphi$, and $k'_\perp$, respectively.

Band in the OC spectrum caused by SCLP photodissociation can also be calculated based on expression (10). The real part of the conductivity has the following form[30]:

$$\mathrm{Re}\,\sigma=\frac{\hbar\Omega N_p\sum_\nu W(\Omega,\nu)}{\varepsilon_\infty E^2}.\tag{16}$$

Here, $W(\Omega,\upsilon)$ is the probability [Eq. (10)] integrated over angular variables where the modulus of the carrier wave vector $k(\varepsilon)$ is expressed as a function of photon energy $\hbar\Omega$ and of the radiated phonon number ν according to expression (9), N_p is the polaron concentration, and the fact that polarons interact with the light in a medium with a refraction index $\sqrt{\varepsilon_\infty}$ is taken into account. By using the expression for β in the Pekar[27] wave function [$\beta=m^*e^2/(2\hbar^2\varepsilon^*)$], one obtains

$$\mathrm{Re}\,\sigma=\frac{1024}{21}\frac{e^2N_p}{m^*\Omega\sqrt{\varepsilon_\infty}}\sum_\nu\left[0.3\varepsilon(\Omega)\frac{\varepsilon^{*2}}{m^*/m_e}\right]^{3/2}\times\left[1+0.3\varepsilon(\Omega)\frac{\varepsilon^{*2}}{m^*/m_e}\right]^{-6}P_\nu$$

or

$$\mathrm{Re}\,\sigma=\frac{1024}{21}\frac{e^2N_p}{m^*\Omega\sqrt{\varepsilon_\infty}}\sum_\nu\left[\varepsilon(\Omega)\frac{0.44}{E_p}\right]^{3/2}\times\left[1+\varepsilon(\Omega)\frac{0.44}{E_p}\right]^{-6}P_\nu,\tag{17}$$

where $\varepsilon(\Omega)$ is determined by expression (9).

III. DISCUSSION OF THE RESULTS AND COMPARISON WITH OTHER MODELS AND WITH EXPERIMENTS

Figures 1 and 2 show the ARPES spectra calculated by expression (15), which are caused by the photodissociation of SCLP with binding energies of 0.17 and 0.14 eV, respectively, at $k_y=0$, $k_x=1$ in π/a units, where a is the lattice constant. For both figures, the electron-phonon interaction constant $\alpha=6$ (it determines the phonon energy for a given

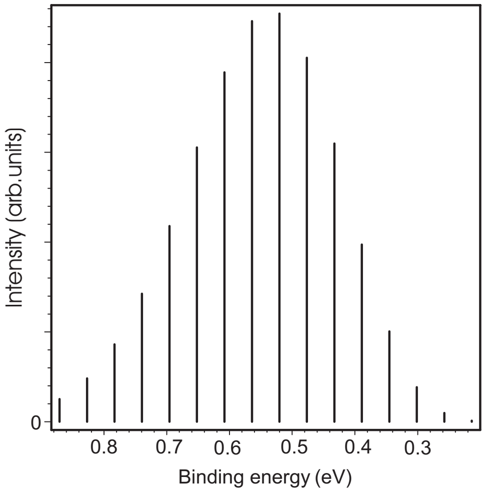

FIG. 1. Band in the ARPES spectrum caused by photodissociation of SCLPs calculated according to expression (15) with $E_p=0.17$ eV at $k_x=1$, $k_y=0$ in neglect of phonon dispersion at $\alpha=6$ (that corresponds to the phonon energy $\hbar\omega=0.044$ eV) and $\hbar\Omega-\Phi=20$ eV.

E_p), $\hbar\Omega-\Phi=20$ eV, and phonon dispersion is neglected. The abscissa axis is in units of the so-called binding energy of electrons in the material,[1,2] i.e., the difference between $\hbar\Omega-\Phi$ and the kinetic energy of photoemitted electrons.

As shown in Figs. 1 and 2, the band calculated with neglected phonon dispersion consists of lines, where each line corresponds to a certain number of radiated phonons. If we do not neglect the phonon dispersion or if we take into account the finite lifetime (ω^{-1}) of the charge carrier in a plane-wave (final) state, the lines in Figs. 1 and 2 will transform into bands, and the resulting summarized band can be structured or unstructured depending on the phonon dispersion (since a distance between neighboring lines comprising the band is the phonon energy). As shown in Figs. 1 and 2, the band in the ARPES spectrum caused by SCLP photodissociation is wide. Its half-width (full width at half height) is in the interval $1.3-1.7E_p$ depending on the phonon energy or the value of α. (The half-width is $1.7E_p$ for $\alpha=6$ and is smaller for larger α.) The band maximum is approximately situated at the electron energy $\hbar\Omega-\Phi-3.2E_p$ or at the binding energy $3.2E_p$.

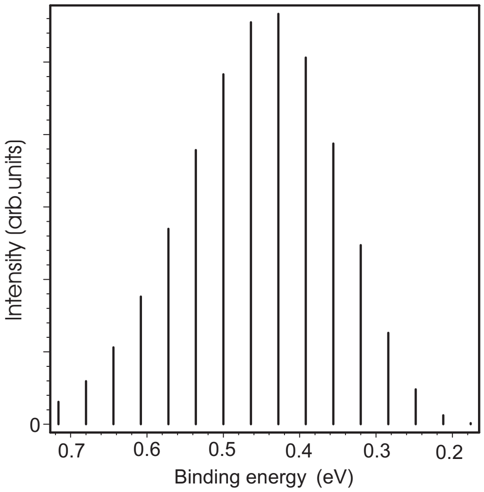

FIG. 2. Band in the ARPES spectrum caused by photodissociation of SCLPs calculated according to expression (15) with $E_p=0.14$ eV at $k_x=1$, $k_y=0$ in neglect of phonon dispersion at $\alpha=6$ (that corresponds to the phonon energy $\hbar\omega=0.036$ eV) and $\hbar\Omega-\Phi=20$ eV.

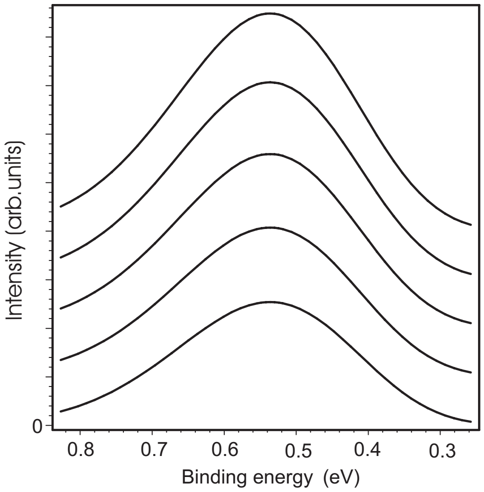

FIG. 3. Energy dispersion curves (their envelopes) calculated by expression (15) for $E_p=0.17$ eV at $\alpha=6$ and $\hbar\Omega-\Phi=20$ eV. Curves from the bottom to the top correspond to $k_y=0$, $k_x=0,0.25,0.5,0.75,1$ in π/a units, respectively.

Figure 3 shows energy dispersion curves (their envelopes) calculated by expression (15) for $k_y=0$, k_x changing from 0 up to 1 (in π/a units). As shown in Fig. 3, the position of the maximum in the $T=0$ K limit does not depend on the electron wave vector direction. This result is opposite to the case of small polarons calculated in the *t-J* model,[3,18] wherein the band in the ARPES spectrum caused by polarons shows dispersion similar to the carrier dispersion in the *t-J* model without phonons. As shown in Fig. 3, the intensity of the band in the ARPES spectrum caused by SCLP photodissociation depends on the in-plane wave vector value in accordance with scalar product expression (14). Namely, the band intensity changes two times with the wave vector k_x changing from 0 up to π/a at $k_y=0$. Approximately, the same change in intensity is shown by the band when the wave vector changes along the diagonal direction.

It is worth noting that the intensity of the so-called coherent zero-phonon line (band) is equal to zero in the $T=0$ K limit. The reason for this, as discussed above, is as follows: if the number ν of radiated phonons is zero, then the total wave vector of radiated phonons is $\mathbf{q}_0=0$. Hence, according to the momentum conservation law in the $T=0$ K limit, $\mathbf{k}=\mathbf{Q}$ and $\mathbf{kA}=\mathbf{QA}=0$, i.e., the probability [Eq. (10)] of a transition with the appearance of $\nu=0$ phonons is zero in the $T=0$ K case.

We calculate the band in ARPES and OC spectra caused by SCLP photodissociation by considering a three-dimensional (3D) medium. Nevertheless, the result can be compared to experimental spectra in effectively two-dimensional (2D) cuprates since the difference between the 3D and 2D cases in such calculation is small, as shown by

TABLE I. Position of the maximum $E_{\max}$ of band in the ARPES spectrum experimentally observed in different materials and polaron binding energies E_p calculated from them.

Material	$E_{\max}$ (eV)	E_p (eV)
$La_{2-x}Sr_xCuO_4$ ($x=0,0.03$)	≈ 0.48 [a]	≈ 0.15
$Nd_{2-x}Ce_xCuO_4$ ($x=0.04$)	≈ 0.39 [b]	≈ 0.122
$Ca_{2-x}Na_xCuO_2Cl_2$ ($x=0,0.05$)	≈ 0.5 [c]	≈ 0.156
La_2CuO_{4+y}	About 0.5[d]	≈ 0.156

[a] Reference 4.
[b] Reference 5.
[c] Reference 6.
[d] Reference 3.

Emin.[22] Comparison of the band in the ARPES spectrum due to SCLP photodissociation calculated according to expression (15) with experimental ARPES spectra of underdoped cuprates shows good conformity: experimental spectra contain broad bands with the maximum at the carrier binding energy $E_{\max}$ shown in the second column of Table I. The third column of Table I shows the binding energies of SCLPs that can cause such bands, which are calculated as $E_{\max}/3.2$ according to expression (15). The values of these binding energies and corresponding phonon energies are quite typical for strong-coupling large polarons in cuprates and other complex oxides.

Indeed, the adiabatic condition determining the strong-coupling case requires the polaron binding energy to be much higher than the phonon energy; the electron-phonon coupling constant is $\alpha \gtrsim 6$. It corresponds to the average phonon number, $\bar{\nu}=2E_p(\hbar\omega)^{-1} \gtrsim 7.77$. The phonon energy corresponding to these parameters is $\hbar\omega=2E_p/\bar{\nu} \lesssim E_p/3.89$. The values of phonon energy corresponding to the polaron binding energies from the third column of Table I are in good conformity with experimental data for cuprates. For example, the phonon branches strongly interacting with the charge carrier in $Nd_{1.85}Ce_{0.15}CuO_4$ have the frequencies of 115, 130, 146, 220, and 305 cm^{-1}.[31] The energies of phonons strongly interacting with the charge carrier in copper-containing complex oxides were also estimated based on the experimental data in Ref. 32 as the value of the order of 0.02 eV.

The form of the bands calculated according to expression (15) is also in good conformity with the experiments. The half-width of the experimental band estimated from its lower binding energy part as in Ref. 3 and half-width of the band calculated according to expression (15) are close. However, the experimentally measured edge of the band from the higher binding energy side is essentially enhanced in comparison with the lower binding energy part.[3] Different mechanisms of carrier scattering at crossing the crystal that we do not take into account in our calculation can be responsible for this effect.

As we use the common approach to calculate bands due to SCLP photodissociation in ARPES and OC spectra, we obtain them in terms of the same parameters—polaron binding energy E_p and phonon energy. Therefore, one can predict the position of the maximum and the form of the band in the ARPES spectrum based on the maximum position of the OC mid-IR band and vice versa. To do it, let us consider the band in the OC spectrum caused by SCLP photodissociation determined by expression (17).

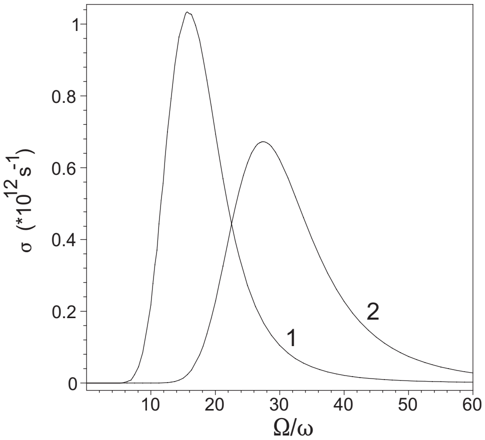

FIG. 4. Optical conductivity $\sigma/(\sqrt{\varepsilon_\infty}m^*/m_e)$ caused by photodissociation of Landau–Pekar polarons at their concentration, $N_p=10^{18}$ cm^{-3}. Curve 1 corresponds to $\alpha=6$ ($\bar{\nu}=7.776$, $E_p=0.1125$ eV if $\hbar\omega=0.03$ eV). Curve 2 corresponds to $\alpha=8$ ($\bar{\nu}=13.824$, $E_p=0.207$ eV if $\hbar\omega=0.03$ eV). The abscissa axis is in units of the ratio of photon frequency to phonon frequency.

An example of these bands is shown in Fig. 4 for $\alpha=6$ (curve 1) and $\alpha=8$ (curve 2) that corresponds to $E_p=0.117$ eV and $E_p=0.207$ eV, respectively, if the phonon energy $\hbar\omega=0.03$ eV. More precisely, Fig. 4 shows $\sigma(\Omega)/[\sqrt{\varepsilon_\infty}(m^*/m_e)]$ for a system with the polaron concentration $N_p=10^{18}$ cm^{-3}. Since expression (17) represents the optical conductivity linear in the polaron number approximation, one can easily obtain the spectra for any other polaron concentration. As shown in Fig. 4, the absorption band due to SCLP photodissociation turns out to be unstructured. It is natural as the band consists of “partial“ bands, each partial band corresponds to a certain value of number ν of radiated phonons. The distance between neighbor partial bands is $\hbar\omega$, whereas the width of each partial band is determined by the condition $kR<1$, where R is the polaron radius[22] (while the condition is satisfied, the matrix element is significant) and is of the order of E_p.[22] According to the adiabatic condition satisfied in the strong-coupling case, $E_p \gg \hbar\omega$; hence, the band is unstructured.

As shown in Fig. 4, the optical conductivity band caused by the SCLP photodissociation is a wide band with a maximum at $\Omega_{\max}\approx 4.1 \div 4.2 E_p/\hbar$, a half-width $\Delta\Omega \approx 2.2 \div 2.8 E_p/\hbar$ (in case of $\alpha=6-8$), and a long-wavelength edge $\Omega_{\text{edge}}=E_p/\hbar+\omega$, as $\nu \gtrsim 1$. Increase in the polaron binding energy results in an increase in $\Omega_{\max}$ and $\Delta\Omega$ (curve 2). However, being expressed in units of $E_p/\hbar$, the value $\Omega_{\max}$ remains unchanged, $\Omega_{\max}\approx 4.2E_p/\hbar$, whereas $\Delta\Omega$ even decreases from $2.8E_p/\hbar$ to $2.2E_p/\hbar$ as α increases. Thus, in the case of $\alpha=6-8$, one can calculate the polaron binding energy from its absorption spectrum as $E_p=\hbar\Omega_{\max}/4.2$.

It is useful to compare the band in the OC spectrum due to SCLP photodissociation calculated at classical[22] and at quantum-mechanical consideration of the polarization field.

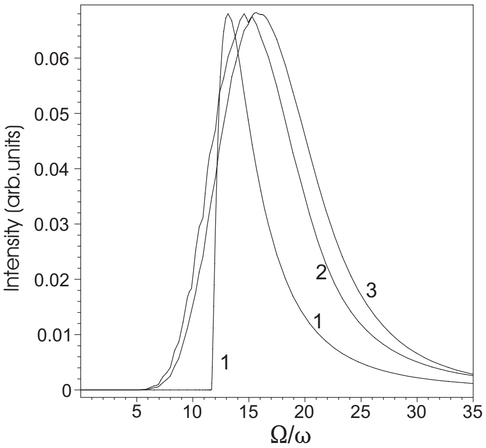

FIG. 5. Light absorption caused by photodissociation of SCLPs. Curve 1 is calculated according to Ref. 22 and curves 2 and 3 are calculated by expression (17) with the Emin (Ref. 22) and Pekar (Ref. 27) wave functions of the charge carrier in the polaron, respectively. For all the curves, $\bar{\nu}=7.776$ (i.e., $\alpha=6$), $E_p=0.1125$ eV, the phonon energy $\hbar\omega=0.03$ eV. The abscissa axis is in units of the ratio of photon frequency to phonon frequency.

Curve 1 in Fig. 5 is calculated according to the Emin[22] expression, curve 2 is calculated by expression (17) but with the carrier wave function in the polaron used by Emin,[22] and curve 3 is calculated by expression (17) with the Pekar[27] wave function of the carrier in the polaron. As shown in Fig. 5, the spectrum obtained in the present work essentially differs from that predicted by Emin.[22] They differ in the low-frequency edge position: $\hbar\Omega_{\text{edge}}=3E_p$ in Ref. 22 and $\hbar\Omega_{\text{edge}}=E_p+\hbar\omega$ in the present work. In the band maximum position, $\hbar\Omega_{\max}=3-3.5E_p$ in Ref. 22and $\hbar\Omega_{\max}=4.2E_p$ in the present work. In the half-bandwidth of the band, $\hbar\Delta\Omega\approx 1.5E_p$ in Ref. 22 and $\hbar\Delta\Omega=2.2-2.8E_p$ in the present work. The band obtained in the present work is more symmetrical with a stretched low-frequency tail apart from the high-frequency one.

Thus, the OC band caused by the SCLP photodissociation is a wide unstructured band with a single maximum at the frequency $\Omega_{\max}\cong 4.2E_p/\hbar$ and a half-bandwidth of the order of $2.2-2.8E_p/\hbar$ (in the case of $\alpha=6-8$). It is natural to compare this band to mid-IR bands observed in the OC spectra of nonstoichiometric (doped to obtain excess charge carriers) complex oxides: cuprates[7–16] and nikelates.[17] The maxima of mid-IR bands in the OC spectra of complex oxides are shown in the second column of Table II. The values of E_p calculated for these substances from the band maximum positions $\hbar\Omega_{\max}$ according to the result of the present consideration as $\hbar\Omega_{\max}/4.2$ are shown in the third column of Table II. They are in good conformity with E_p values calculated according to the SCLP theory[26,27] applied to medium parameters typical for complex oxides: $\varepsilon^*\approx 3-4$, $m^*/m_e=1-2$ ($E_p=0.092-0.327$ eV). Obviously, interpretation of these bands as bands caused by carrier transitions into polaronic relaxed excited states calculated in works[24,25] where the energy of the band maximum is about E_p ($E_p\approx\hbar\Omega_{\max}$) results in polaron binding energies that are too large for the large radius polarons. Interpretation of these experimental mid-IR bands caused by SCLP photodissociation does not lead to such contradiction.

TABLE II. Maximum position of mid-IR bands in the OC spectrum experimentally observed ($\hbar\Omega_{\max}^{\text{photodiss}}$ is the maximum of the high-frequency mid-IR band and $\hbar\Omega_{\max}^{\text{internal}}$ is the maximum of the low-frequency mid-IR band) and the polaron binding energy E_p calculated from $\hbar\Omega_{\max}^{\text{photodiss}}$.

Material	$\hbar\Omega_{\max}^{\text{photodiss}}$ (eV)	E_p (eV)	$\hbar\Omega_{\max}^{\text{internal}}$ (eV)
$Yba_2Cu_3O_{6+y}$	0.62 ± 0.05 [a]	$\approx 0.155\pm0.01$	0.16 ± 0.03 [a]
Nd_2CuO_{4-y}	0.76 ± 0.01 [a]	≈ 0.18	0.162 ± 0.005 [a]
$La_{2-x}Sr_xCuO_{4+y}$	0.53 ± 0.05 [a]	$\approx 0.126\pm0.01$	0.16 ± 0.03 [a]
La_2CuO_{4+y}	0.6 ± 0.02 [a]	$\approx 0.143\pm0.005$	0.13 ± 0.02 [a]
$Nd_{2-x}Ce_xCuO_4$ ($x=0.05$)	0.55[b]	≈ 0.131	0.11[b]
$Nd_{2-x}Ce_xCuO_4$ ($x=0.1$)	0.39[b]	≈ 0.093	0.09[b]

[a] Reference 14.
[b] Reference 15.

However, the bands caused by phototransitions into polaronic relaxed excited states calculated in Refs. 24 and 25 can also be found in the OC spectra of complex oxides. Several groups reported the experimental spectra that pointed out that the mid-IR bands in the OC spectra of complex oxides have a complex structure in which two bands can be distinguished.[14–16] Column 4 of Table II shows the maxima of the low-frequency mid-IR bands in experimental OC spectra. If we suppose that these bands are caused by transitions into polaronic relaxed excited states studied in Refs. 24, 25, and 29, then according to Refs. 24 and 25, their maxima are located at approximately E_p. Comparison of the polaron binding energies, which are calculated from the maximum position of high-frequency mid-IR bands (column 3), with the energies of the maximum of the low-frequency mid-IR bands (column 4) show good agreement of our supposition with the experiment. This can also be seen from the comparison of the ratio $\Omega_{\max}^{\text{photodiss}}/\Omega_{\max}^{\text{internal}}$ obtained from the experimental OC spectra,[14–16] $\Omega_{\max}^{\text{photodiss}}/\Omega_{\max}^{\text{internal}}=4-4.5$, with that predicted by united results of the present work and those of Refs. 24 and 25: $\Omega_{\max}^{\text{photodiss}}/\Omega_{\max}^{\text{internal}}\cong 4.2$.

Thus, the presence of two bands in the OC spectrum of complex oxides is in good conformity with the predictions of the SCLP theory. The form of the high-frequency mid-IR bands in complex oxides is also in good conformity with that calculated by expression (17). It is shown in Fig. 6, wherein we fitted the experimental OC spectrum[14] using expression (17). The width of the band theoretically calculated would be larger if we took into account the limitation of the wave vector space in the first Brillouin zone. Besides, we calculate the band for the case of medium with a single phonon branch strongly interacting with the charge carrier, whereas in complex oxides, ordinarily, there are several such branches. Taking into account this fact will lead to a variety of the band forms. Allowing for interaction of polarons will also likely lead to broadening of the band as it occurs in the weak-coupling case.[33]

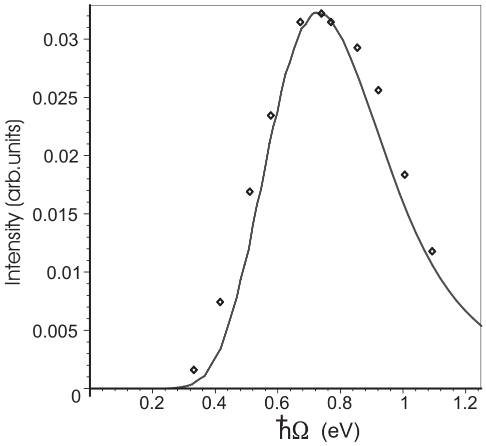

FIG. 6. Mid-infrared band in the optical conductivity spectrum of Nd_2CuO_{4-y} (Ref. 14) at temperature $T=10$ K (diamonds) and its fit by expression (17) with $\alpha=6$, $E_p=0.18$ eV (solid curve).

Now, let us compare the polaron binding energies calculated from the experimentally observed band in the ARPES spectrum (as $E_{\max}/3.2$) to that from the mid-IR band in the OC spectrum (as $\hbar\Omega_{\max}/4.2$). They are presented in Table III. Unfortunately, we are not aware of both ARPES and OC spectra for a material with precisely the same doping level only for somewhat different doping levels. This can lead to worse coincidence since the polaron binding energy and the maximum position of the bands depend on the doping level, as will be discussed in Sec. IV. Nevertheless, as shown in Table III, the polaron binding energies E_p calculated from the ARPES and OC spectra for the same material with a close doping level show good agreement (the difference is within 10%). Hence, the approximation of the final carrier states with plane waves used in the calculation of the OC band caused by SCLP photodissociation, as discussed in Sec. I, does not lead to a large error and can be applied.

Thus, the result of the present consideration allows us to predict the position of the maximum of the band in the ARPES spectrum based on the maximum position of the mid-IR band in the OC spectrum (using a factor of 3.2/4.2) and vice versa. An example of such prediction is demonstrated in Table IV. The second column of Table IV contains the maxima of mid-IR bands experimentally obtained in Refs. 7–13 and collected together in Ref. 34. The third column of Table IV shows the binding energy of SCLPs calculated from the maximum positions. The fourth column of Table IV shows the predicted positions of the maximum of the bands in the ARPES spectrum (the carrier binding energy in eV) in these materials.

IV. INFLUENCE OF TEMPERATURE AND CARRIER CONCENTRATION ON ANGLE-RESOLVED PHOTOEMISSION SPECTROSCOPY AND OPTICAL CONDUCTIVITY SPECTRA CAUSED BY STRONG-COUPLING LARGE POLARONS

We calculate the bands in the ARPES and OC spectra caused by SCLP photodissociation in the $T=0$ K approximation, i.e., for resting or moving slowly (with the velocities considerably lower than the maximum group velocity of phonons interacting with the carrier) polarons. Influence of the temperature on the bands will naturally lead to an increase in their width. However, the theory of photodissociation of SCLPs in the case of nonzero temperatures is essentially complicated. Coherent polarization in SCLP cannot propagate with a velocity higher than the group velocity of phonons participating in the polaron formation.[18,35] In the case considered by Pekar[27] and in the present work, we use the model with dispersionless phonons that corresponds to zero velocity of phonons. In such a model, one cannot consider the thermal motion of polarons. Besides, the distribution function of polarons has peculiarities caused by competition of polaron and Bloch states of a charge carrier.[36,37] The problem of ARPES and OC spectra of SCLPs at finite temperatures will be considered elsewhere.

However, we can predict the change in the integral intensity of bands in the ARPES and OC spectra caused by SCLP photodissociation with the temperature. The characteristic feature of the SCLP is the limitation of its velocity by the maximum group velocity of phonons participating in its formation.[35] It results in the thermal destruction of the SCLPs when their thermal velocities exceed the minimum phase velocity of relevant phonons. The thermal destruction expresses itself in a gradual decrease in the polaron concentration with temperature at critical temperatures much lower than E_p. (The critical temperature is determined by the values of the phonon maximum group velocity and the polaron binding energy.[36,37]) Therefore, the integral intensity of the

TABLE III. Comparison of binding energies of SCLP estimated from the ARPES and OC spectra.

Material with measured ARPES spectrum	E_p calculated from ARPES spectrum (eV)	Material with measured OC spectrum	E_p calculated from OC spectrum (eV)
$Nd_{2-x}Ce_xCuO_4$ ($x=0.04$)	≈0.122 eV [a]	$Nd_{2-x}Ce_xCuO_4$ ($x=0.05$)	≈0.131 eV [b]
$La_{2-x}Sr_xCuO_4$ ($x=0,0.03$)	≈0.15 eV [c]	$La_{2-x}Sr_xCuO_{4+y}$	≈0.126±0.01 eV [d]
La_2CuO_{4+y}	≈0.156 eV [e]	La_2CuO_{4+y}	≈0.143±0.005 eV [d]

[a] Reference 5.
[b] Reference 15.
[c] Reference 14.
[d] Reference 4.
[e] Reference 3.

TABLE IV. Experimentally observed maximums of mid-IR band in OC spectrum of different materials and predicted position of maximum of band in ARPES spectrum.

Material	Maximum of mid-IR band in OC spectrum (eV)	Binding energy of the polaron (eV)	Predicted position of maximum of band in ARPES spectrum (eV)
$Bi_2Sr_2CaCu_2O_8$ (a axis)	0.545[a]	0.129	0.415
$Bi_2Sr_2CaCu_2O_8$ (b axis)	0.51[a]	0.121	0.388
$La_{1.9}Ca_{1.1}Cu_2O_{6+\delta}$	0.59[b]	0.14	0.45
$La_{1.85}Sr_{0.15}CaCu_2O_{6+\delta}$	0.57[b]	0.136	0.43
$La_{1.9}Sr_{0.1}CuO_{4+\delta}$	0.46[c]	0.109	0.35
$YBa_2Cu_4O_8$	0.55[d]	0.13	0.42
$HgBa_2CuO_{4+\delta}$	0.48[e]	0.114	0.366
$Bi_2Sr_2Ca_2Cu_3O_{10}$	0.63[f]	0.15	0.48
$YBa_2Cu_4O_{6.9}$	0.65[g]	0.155	0.495

[a] Reference 7.
[b] Reference 8.
[c] Reference 9.
[d] Reference 10.
[e] Reference 11.
[f] Reference 12.
[g] Reference 13.

band will decrease with the increase in temperature.

An example of the polaron thermal destruction at temperatures low in comparison with the polaron binding energy is represented by the optical conductivity spectrum of β-$Na_{0.33}V_2O_5$.[38] It contains a mid-IR band with the maximum at 3000 cm^{-1} that can be caused by the photodissociation of SCLP with a binding energy of about 0.09 eV. [Indeed, the form of the band in the low-temperature spectrum ($T=5$ K) is in good conformity with its fit by expression (14) with $E_p=0.089$ eV, $\alpha=6$. The phonon energy corresponding to these parameters ($\hbar\omega=2E_p/\bar{\nu}=0.025$ eV) is in good conformity with the reflectivity spectra,[38] demonstrating a large longitudinal-transverse splitting (i.e., strong electron-phonon interaction) for a set of phonon branches with frequencies of 80–300 cm^{-1}.] Already the optical conductivity spectrum of β-$Na_{0.33}V_2O_5$ corresponding to $T=145$ K shows a decrease in the integral intensity of the mid-IR band, and the 300 K spectrum shows an approximately two times lower integral intensity in comparison with that for the $T=5$ K spectrum.[38] A similar decrease in the integral intensity of the mid-IR band in the OC spectrum is shown by $Nd_{2-x}Ce_xCuO_4$.[15]

Transition of the charge carriers from the polaron states into the free carrier states with increasing temperature also results in the essential lowering of their effective mass. Therefore, some decrease in the system resistance (the so-called activational behavior) may occur in the corresponding temperature interval[37] if the change in the carrier relaxation time at the transition will not compensate this effect. Some complex oxides demonstrate such a behavior of the system resistance and Hall coefficient.[15,39] For example, the integral intensity of the mid-IR band in the OC spectrum of $LaTiO_{3.41}$ decreases by three to four times in the region with temperatures of 150–300 K.[39] In the same temperature region, the resistance along the direction $\parallel a$ shows the change in its temperature behavior: in the region of 50–150 K, the resistance increases with the temperature increase, whereas in the region of 150–300 K, the increase stops and the resistance remains practically constant with increasing temperature. It is in conformity with the temperature behavior of resistance in systems with SCLPs.[37]

We calculate the bands in the ARPES and OC spectra in the limit of noninteracting polarons so that our results are valid only in the case with a low carrier concentration (small doping level). However, based on carrier distribution function in systems with strong-coupling polarons,[36] we can predict some consequences of the increase in the carrier concentration. According to the carrier distribution function in systems where SCLP can form,[36] free charge carriers coexist with polarons at nonzero temperatures or at carrier concentration higher than the maximum polaron concentration, $n_0=2V_0^{-1}$, where V_0 is the polaron volume. Therefore, already at the doping level higher than approximately 0.03, one can expect in the ARPES spectrum features caused by free charge carriers together with those caused by polarons. Besides, screening of the electron-phonon interaction by free charge carriers will cause a decrease in the polaron binding energy and, consequently, a decrease in the energy corresponding to the mid-IR band maximum at the increase in doping, as demonstrated by the experiment.[15]

V. CONCLUSION

Thus, according to the result of the present consideration, the band in the ARPES spectrum caused by SCLP photodissociation is a wide nondispersing band with the maximum approximately at a binding energy of $3.2E_p$ and the half-width of about $1.5E_p$. According to the carrier distribution function in the system with SCLPs,[36] free charge carriers coexist with polarons already at the doping level higher than 0.03. One can expect corresponding features in ARPES spectrum together with the band caused by SCLP photodissociation. In the OC spectrum, SCLP photodissociation results in the band with a maximum at approximately $4.2E_p$ and the half-width of about $2.5E_p$. However, together with it and the Drude contribution, the OC spectrum of SCLPs contains another band caused by transitions into polaronic relaxed excited states (states of discrete energy spectrum). According to Refs. 24 and 25, the maximum of this band is situated at approximately E_p. Bands in the ARPES and OC spectra caused by SCLP photodissociation are wide, which is in conformity with experiment, as the method suggested allows us to describe the appearance of many phonons in a single act of SCLP photodissociation (different numbers of phonons in different acts).

The common approach used to calculate bands in the ARPES and OC spectra caused by SCLP photodissociation allows the coordinated interpretation of the ARPES and OC spectra of complex oxides. By using the results of the present consideration, one can predict the position of the maximum and half-width of the band in the ARPES spectrum from the position of the maximum of the mid-IR band in the OC spectrum and vice versa. By comparing the results of the present consideration with experiments, we can conclude that underdoped cuprates contain SCLPs. The values of the polaron binding energy calculated according to expressions (15) and (17) from the ARPES and OC spectra of the same material are in good conformity: the difference between them is within 10%. This confirms the applicability of the supposition made that plane-wave states can be used for the approximation of final carrier states in the calculation of the OC band caused by SCLP photodissociation.

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